Data-driven Numerical Methods for Kernel Matrices

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Abstract

Kernel matrices play a pivotal role in various machine learning and scientific applications, with their structure critically influenced by both the parameters of the kernel function and the data distribution [2]. This talk will begin with a geometric analysis of the Schur complement of the kernel matrix, examining the effects of kernel bandwidth and data distribution on its structure. Building on these geometric insights, we design the Adaptive Factorized Nyström (AFN) preconditioner [1] for solving linear systems associated with the regularized kernel matrix. The AFN preconditioner enhances the Nyström approximation by constructing a sparse approximate inverse for the Schur complement, significantly improving robustness and efficiency across a wide range of parameters. Finally, we will introduce HiGP [4], a high-performance Python package designed for Gaussian Process Regression (GPR) and Classification (GPC). HiGP integrates AFN and some preconditioned iterative methods [3] to boost the efficiency and scalability of model training and inference across various datasets.

References

[1] S. Zhao, T. Xu, H. Huang, E. Chow, and Y. Xi, *An Adaptive Factorized Nyström Preconditioner for Regularized Kernel Matrices*, SIAM J. Sci. Comput., 46(4), (2024), A2351-A2376.

[2] D. Cai, H. Huang, E. Chow, and Y. Xi, *Data-Driven Construction of Hierarchical Matrices With Nested Bases*, SIAM Journal on Scientific Computing, 46(2), (2024), S24-S50.

[3] D. Cai, E. Chow, and Y. Xi, *Posterior Covariance Structures in Gaussian Processes*, arXiv preprint arXiv:2408.07379.

[4] H. Huang, T. Xu, Y. Xi, and E. Chow, *HiGP: High-Performance Python Package for Gaussian Process Regression*, Retrieved from https://github.com/huanghua1994/HiGP